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FINITE ELEMENT MODELING OF COUPLED HEAT AND MOISTURE
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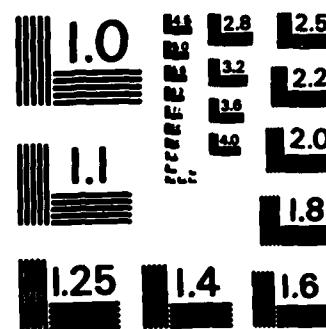
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The purpose of this research was to investigate the use of finite element techniques for solving convective heat transfer problems which involve phase change. The specific application was to permafrost modeling. This has been accomplished at several levels, ranging from very theoretical error estimates and development of special numerical techniques to handle phase change, to application of finite element techniques to specific permafrost problems.			

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SUMMARY

The purpose of this project was to investigate the use of finite element techniques for solving convective heat transfer problems which involve phase change. The specific application was to permafrost modeling. This project has been accomplished at several levels, ranging from very theoretical error estimates and development of special numerical techniques to handle phase change, to application of finite element techniques to specific permafrost problems. Our research has focused on the following areas:

- (1) Analysis of convective effects in convection-diffusion processes;
- (2) Use and analysis of upwinded finite elements to stabilize convection-diffusion models in the presence of layers and fronts;
- (3) Error analysis of moving meshes to track a time-dependent freeze front;
- (4) Special techniques to track the freeze front and to accurately calculate the energy contribution due to the latent heat of fusion during phase change.
- (5) Error estimates for the finite element alternating-direction procedures developed here;
- (6) Basic questions relating to the numerical solution of general heat transfer processes.

DISCUSSION

An eigenvalue analysis [1,4] was used to study the theoretical properties of general convection-diffusion problems. The specific structure of the semidiscrete systems obtained by alternative finite element methods are analyzed using Gershgorin theory and the theory of oscillation matrices. This provided an interesting approach for analyzing the effects of higher-order elements, upwinding and mesh refinement. This provided a better understanding of oscillatory and dissipative effects artificially introduced by particular numerical models. We have also investigated freezing in the presence of internal convection [16,22,23]. We have found that one can control oscillations, in this case, to some degree, by varying the mesh size and element placement. In some related studies we have examined the effect of different boundary conditions on the development of oscillations due to a discontinuity in the initial data and reflection of a front at a boundary [9]. Both dissipative backward-type integration schemes and nondissipative central schemes have been used in a comparative numerical studies. The algorithms are based on variable order - variable step integration techniques.

One of the major difficulties in dealing with transport problems in which convection plays an important role is the effective treatment of sharp fronts in the solution profiles. Some techniques, although accurate, lead to oscillatory errors while others are over-dissipative. In our investigations of these problems we have developed a class of upwind finite element methods in which the amount of upwinding is controlled adaptively during the solution procedure [1].

The eigenvalue analysis in [4] forms the basis of this new method for variable upwinding in finite element solution of convection-dominated flows [24]. The approach seems quite general and can be used for non-uniform meshes, a point that has not been generally true of other upwind techniques. We have extended the technique to nonlinear convection-diffusion problems using local linearization in a given timestep to select the local dissipation in the upwinding strategy [9]. Earlier, good results were obtained with linear model problems. Subsequently, we have applied the technique successfully for a multicomponent-multiphase coupled flow, with a sharp front [21]. The scheme is also being used in conjunction with adaptive mesh refinement for problems with sharp layers such as those encountered in the application of interest in our present research [17]. Some related results were presented as an invited paper at the SES meeting in December, 1980.

Quite a bit of progress has been made in the development and analysis of moving mesh techniques for solving heat transfer problems both with strong convection and with mild convective effects. The problem may be viewed as an optimal control problem in which both the solution values and the nodal coordinates for the mesh are to be determined at each timestep.

A fundamental question in the analysis of the permafrost problem and similar problems involving a change of phase is the treatment of the free surface. A significant part of the research effort has been directed towards the implementation of a practical front tracking technique and of accurate latent heat calculations for two-dimensional thawing around a pipe. Numerical calculations are very sensitive to the latent heat contributions, so one must balance the desired accuracy with the computational expense. The front location and latent heat contribution may oscillate when standard time integration techniques are employed. To circumvent this problem a modified predictor-corrector strategy has been developed and implemented in the two-dimensional permafrost code [20]. A series of numerical experiments have been conducted to evaluate and compare these methods with more standard techniques. The difficulties involved with latent heat are more apparent in problems involving several materials and irregular geometries. We investigated the effects of using various sizes of finite elements, different orders of finite elements, and different numbers of elements within a given material property upon the numerical calculations [23,26]. This leads to some general guidelines for setting up finite element grids in irregular geometries when latent heat must be dealt with [25,26].

Error estimates for nonlinear parabolic p.d.e.'s using an alternating-direction technique have been obtained for several numerical algorithms. These algorithms have been compared in terms of execution time, solution accuracy and storage requirements for simple two-dimensional model problems [7,14,5]. This work generalizes the alternating-direction method to general curved geometries using isoparametric finite elements. This technique allows two- and three-dimensional problems to be solved as a series of one-dimensional problems [13,14,6]. These techniques require considerably less computer time and storage

than standard finite difference or finite element methods. We have investigated the use of reduced integration to further improve computational efficiency. This lead to a criteria for the lowest order stable numericr' integration scheme [12,15]. This criteria depends on the differential equation as well as the particular boundary conditions.

Finally, part of our research efforts were directed at a variety of basic questions dealing with numerical solution of complex heat transfer processes, such as in what form should the time-dependent finite element equations be written to insure that the proper interface condition is implemented at material interfaces as well as at ice-water interfaces [19], and what options may one use to implement a convection boundary condition and still maintain numerical stability. Other related work has dealt with the selection of appropriate flux conditions and treatment of the capacity coefficient in the governing equation. One approach to modeling heat transfer in permafrost is to replace the infinite boundary by a finite boundary and to apply the boundary condition at infinity to this finite boundary. This can lead to serious errors if the finite boundary is too close to the source. We have investigated the use of a mixed-type boundary condition at the finite remote boundaries and have found that it produces a great increase in accuracy over applying either a fixed temperature or a no heat flow condition. This will allow more accurate modeling over much smaller physical domains.

Part of our work has dealt with fictitious oscillations that arise in finite element modeling of transport problems. These oscillations occur in the convection terms. Both aspects have been studied and results presented at a recent meeting on numerical methods for heat transfer [17]. With respect to the front oscillations, these difficulties have been overcome by means of a new modified predictor-corrector strategy [20]. Problems with convection are treated using a variable upwind finite element technique which is utilized and demonstrated to be effective in suppressing oscillations, while not inducing excessive dissipation and degrading of the solution [9]. Another source of numerical oscillations is when boundary temperatures are changing faster than heat can be conducted through the soil. We have investigated ways in which one can control these oscillations by varying element size, by placing small elements near the boundary and by varying the range of temperatures over which latent heat is liberated [23]. When transient problems involve sharp solution gradients that propagate through a material interface or through an abrupt change in mesh size, similar difficulties arise. We have considered some prototype transient problems and the effect of different boundary conditions on development of oscillations due to phase errors on contact and reflection of the solution [9]. The effect of different ODE integration techniques on suppression of oscillatory errors was also studied [3,10].

In summary, many important theoretical and practical questions related to efficient and accurate permafrost modeling have been addressed during the course of this three-year contract. The results of this project have been widely disseminated in technical journals and reports and at technical meetings. The investigators have been very productive and have answered many questions related to general convective heat transfer with phase change.

TECHNICAL PERSONNEL

Scientific Personnel Supported by this Project
and Degrees Awarded During this Contract Period

G. F. Carey and L. J. Hayes, Co-Principal Investigators
K. Sephrnoori, Research Associate
T. Plover, Research Assistant
A. Mueller, Research Assistant
B. Jiang, Research Assistant
S. Kim, Research Assistant
P. Kenyon, Research Assistant
Y. Ng, Research Assistant
H. Lee, Research Assistant
M. Tsai, Research Assistant

Y. Ng: Awarded Master's Degree - Engineering Mechanics - August 1981
(Direct Implementation of Latent Heat of Fusion for a Permafrost
Problem)

M. Tsai: Awarded Master's Degree - Engineering Mechanics - August 1981
(Semidiscrete Analysis and Solution of Hyperbolic Heat Conduction
with Reflection at a Boundary)

T. Plover: Awarded Master's Degree - Engineering Mechanics - August 1981
(Transport Phenomena Approximation by the Finite Element Method)

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